

Spin-resolved electron spectroscopy of the OCS molecule

G. Snell¹, B. Langer², M. Martins³, E. Kukk⁴, and N. Berrah¹

¹Western Michigan University, Department of Physics, Kalamazoo, MI 49008

²Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany

³Institut für Experimentalphysik, Freie Universität Berlin, D-14195 Berlin, Germany

⁴Dept. of Physics, Oulu University, 90570 Oulu, Finland

Spin-resolved electron spectroscopy of atoms and molecules can yield valuable information about the dynamics of the photoionization and Auger decay processes as well as about the electronic structure of the samples. Quantum mechanically this information is expressed in terms of the wavefunctions for the initial and final states and the dipole and Coulomb transition matrix elements. A complete set of matrix elements, amplitudes and phase shifts, enables the prediction of all observable parameters of the emission process, such as the angular distribution and spin polarization of the electrons. For this reason, big advancements were made in complete photoionization experiments of atoms in recent years [1].

In contrast, there have been only very few studies of inner-shell photoionization of molecules beyond intensities and angular distributions [2]. A molecular ‘complete experiment’ is much more difficult than the determination of matrix elements for atoms, because of the large number of possible outgoing partial waves. Additionally, the molecular environment can influence the core orbitals of the atoms in the molecule. This can lead to the splitting of energy levels due to vibrations, lower than spherical symmetry of the system, etc.

Recently, Kukk et al. [3] investigated the sulphur 2p photoionization of OCS molecules by high-resolution, angle-resolved electron spectroscopy. They found that the angular distribution parameter β of the two molecular-field-split components of the sulphur 2p_{3/2} line differs significantly at a broad range of photon energies above the 2p threshold. Since the origin of this difference cannot be traced solely by angle-resolved spectroscopy, we measured the spin polarization of the S 2p lines. We used circularly and linearly polarized light of 185-220 eV photon energy from the new elliptical polarization undulator (EPU) beamline of the Advanced Light Source storage ring to carry out this experiment. The spin polarization component measured with linearly polarized light is almost zero for all lines of the spectra. In contrast, in the measurements with circularly polarized radiation the 2p_{1/2} line is almost completely polarized and the molecular field split components of the 2p_{3/2} line show clearly different degree of electron polarization. This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division, of the U.S. Department of Energy.

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Principal investigator: N. Berrah, Department of Physics, Western Michigan University. Email: berrah@wmich.edu. Telephone: 616-387-4955.